Physics 232: Computational Physics, Solutions for the Take-home Final Exam

Problem 1: Olympic Long-Jump

Introduction: This problem is similar to problem 1 in the midterm exam, but now we solve the differential equations using a program (in C++) instead of a numerical math package (MAPLE) or a spreadsheet (Excel). We need to solve a set of two coupled differential equations (for the velocities in the vertical and horizontal directions). These equations are nonlinear, since we include a dissipative term for the air resistance. We use Euler's method to solve the equations.

Solution Method: The program BEAMON.CPP allocates two arrays **vx** and **vy** for the velocities, defines the initial conditions and parameters, and then calls a **void** function **Euler()**, passing the arrays, the number of data points **N**, and the step size **h** as parameters. **Euler()** calls **double** functions **f()** and **g()**, passing the current velocities as parameters, to calculate the accelerations. Once the solution to the differential equations is known, it is stored in a file **veloc.dat**. Next, we integrate the velocities using the trapezoidal rule, see Numerical Recipes in C, Eqn. (4.1.3), and store the positions as a function of time in file **posit.dat**. The parameters (drag constant, air density, mass, and gravitational acceleration) are defined as global variables.

Checks on Solution: It is important to check the accuracy of the solution. This can be done in at least two ways. (i) Check the solution in the absence of air resistance (i.e., **k=0**), where the numerical solution can be compared with the analytical solution for a projectile. See the solution for the mid-term exam. Without air resistance, the jump time is between 0.84 and 0.85 s for a step size of 0.01 s. This is very close to the jump time found from the analytical solution (t=0.846 s), therefore **h=0.01 s** should be a good choice for the step size. (ii) Change the number of points (i.e., the step size **h**). There is little difference in the trajectory for **h=0.01 s** and **h=0.005 s**, therefore **h=0.01 s** seems to be a satisfactory choice.

Results and Discussion:
(1) The velocities v_x and v_y as a function of time t are shown in Figs. 1 and 2 for different values of the drag constant k. As expected, the horizontal velocity (dashed line) is hardly affected for k=0.182, since the horizontal force is small (see Fig. 1). For a ten times larger drag constant (k=1.82 m^2, see Fig. 2), the horizontal velocity drops more rapidly.
(2-4) The trajectories (y versus x) are shown in Fig. 3 for two values of ρ (ρ=0.984 kg/m^3 and ρ=1.968 kg/m^3) and in Fig. 4 for two values of k (k=0.182 m^2 and k=0.364 m^2). The two figures are identical, since the product ρk is proportional to the drag force, therefore doubling one has the same effect as doubling the other. Doubling either reduces the range of the jump by only about 10 cm. Therefore, we can conclude that the thin air in Mexico City has little influence on the range of the jump.

Conclusions:
The two coupled nonlinear first-order differential equations describing the motion of a projectile experiencing air resistance were solved using Euler's method by a C++ program. Air resistance has very little influence on the range of the jump and cannot explain why R. Beamon exceeded the previous world record by over 2.5 feet.

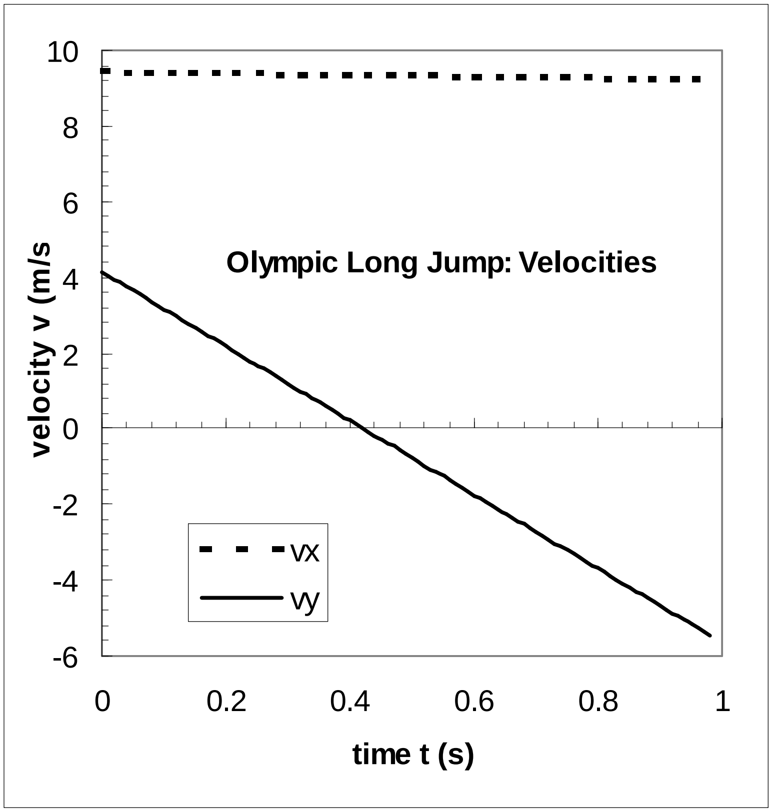

Figure 1: Velocities v_x and v_y as a function of time *t* for *k*=0.182.

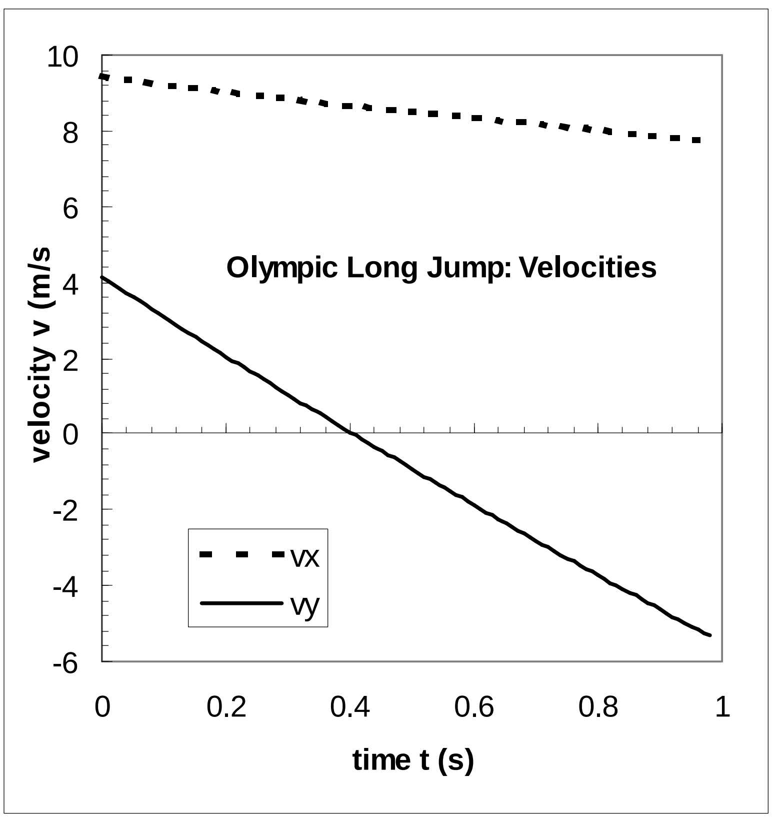

Figure 2: Velocities v_x and v_y as a function of time *t* for *k*=0.1.82.

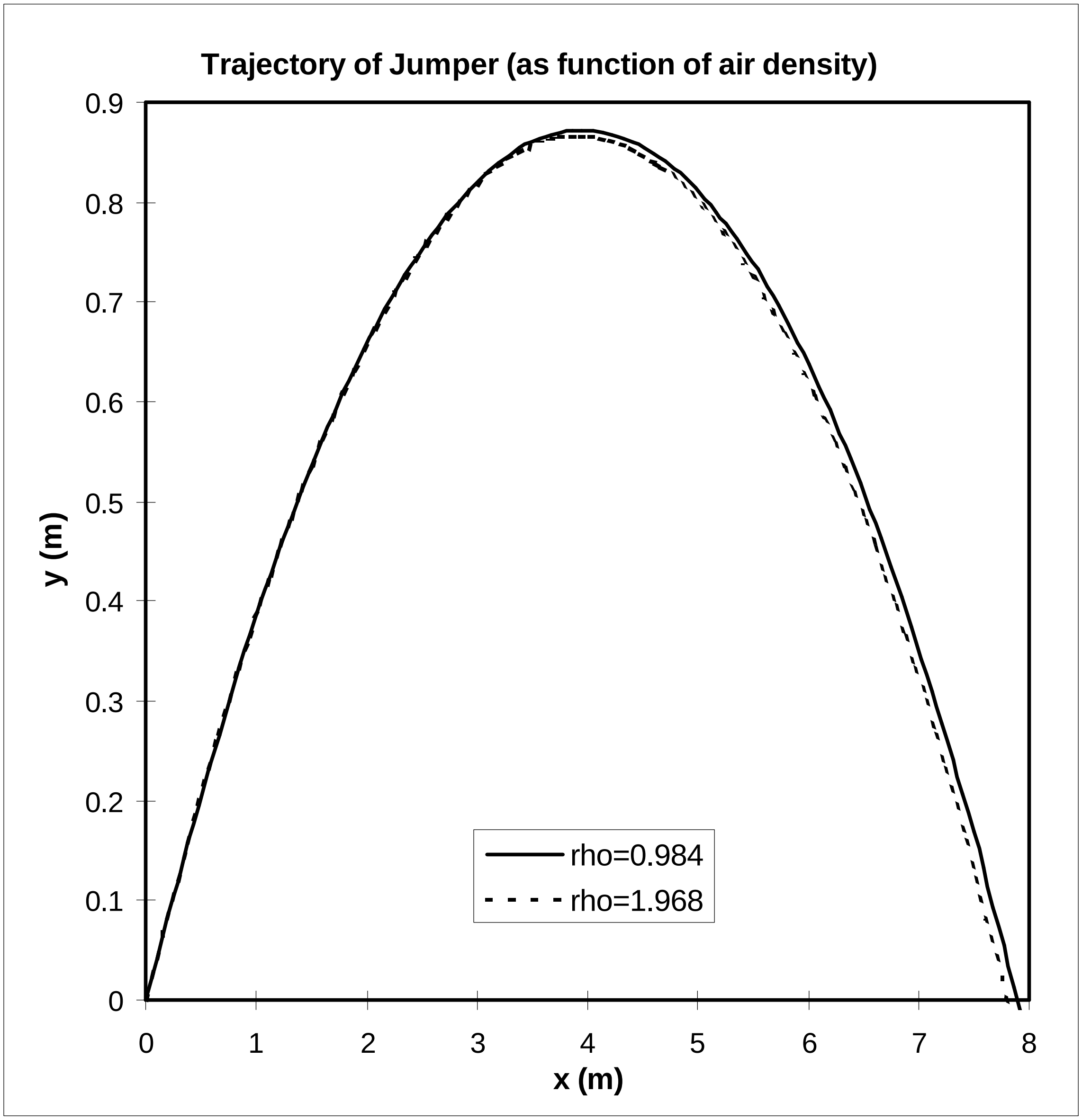

Figure 3: Trajectory (*y* versus *x*) for two different values of ρ.

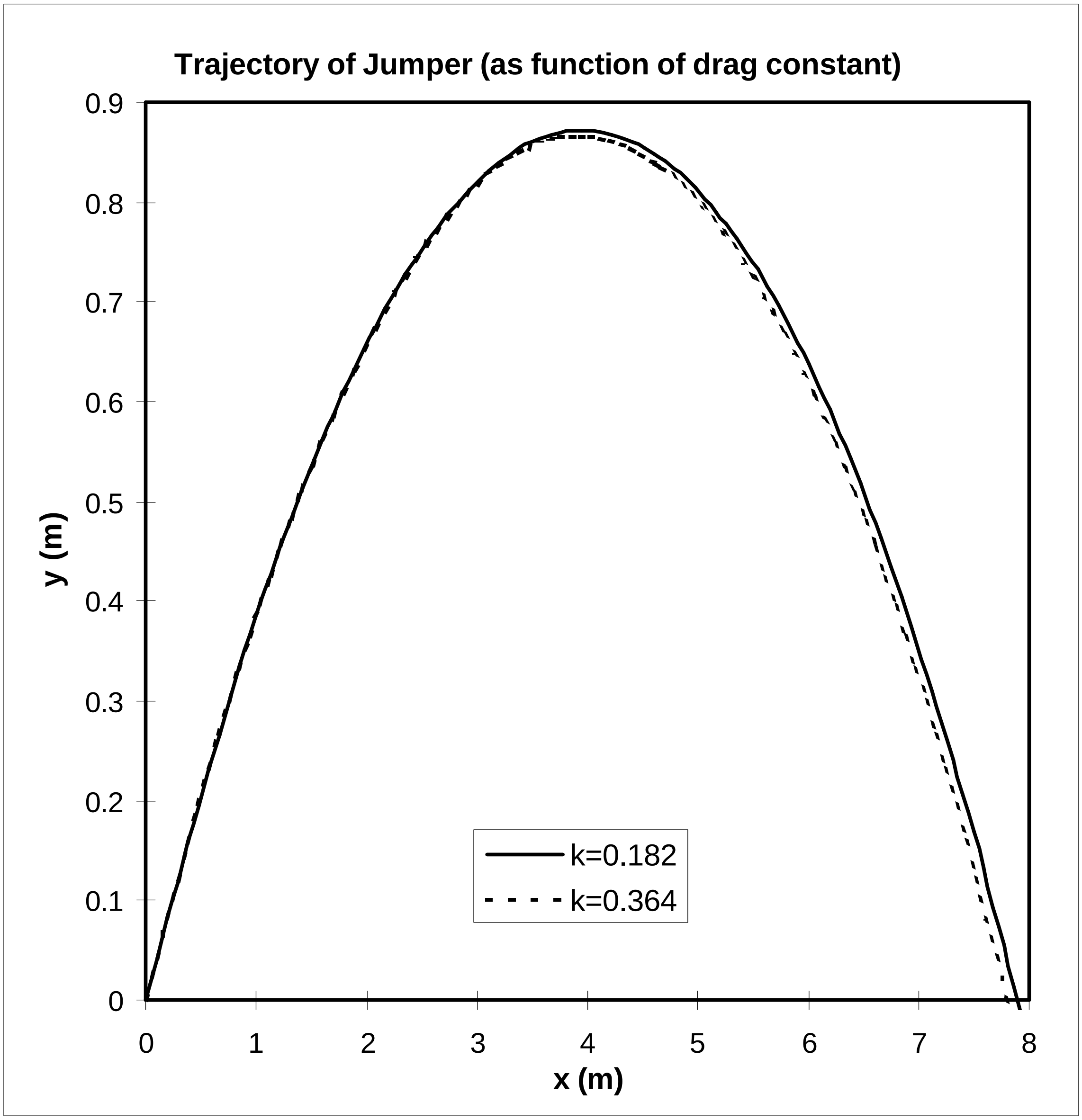

Figure 4: Trajectory (*y* versus *x*) for two different values of *k*.

Problem 2: Quantum Mechanical Particle in a Box

This problem deals with a quantum-mechanical particle in a box. The wave function of this particle needs to solve the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2}+V(x)\Psi=E\Psi$$

When introducing atomic units, where we measure all lengths in Bohr radii and all energies in Hartrees (1 Ha=27.2 eV), we can set $\frac{\hbar^2}{2m}=1$ and the Schrödinger equation becomes equivalent to

$$\frac{d^2\Psi}{dx^2}+[E-V(x)]\Psi=0.$$

Solution Method: This equation can be solved using the shooting method (Numerov algorithm) described in the lab manual (Programming with FORTRAN and/or C). We can use a similar main program as in numerov.cpp. The Numerov() function is also similar, but I have made it more efficient (at least three times faster). Since the function *E-V(x)* is different here, the Numerov() function had to be changed appropriately. There is a second function EmV() which calculates *E-V(x)*. The guess for the energy E and the number of steps are passed as command line parameters. Take a look at the source code to see how the command line arguments are parsed.

Checks on Solutions: We need to verify that the step size is sufficiently small. As usual, we compare with a case that can be sloved analytically, i.e., we remove the bump in the potential. Under these conditions, the wave equation reduces to that for waves on a string. The smallest wavelength we can have for the boundary conditions (wave function is zero on both ends) is $\lambda=2L=2$. For this wavelength, the energy $E=\pi^2$ Ha=9.869 Ha. For a step size of N=100, we obtain the correct energy eigenvalue, therefore the Numerov algorithm seems to be working properly (i.e., the errors are small).

Results and Discussion:

(1) The plot (postscript file) shows the wave with the smallest wavelength for three different magnitudes of the bump. First, we set the height of the bump to zero and plot the solution. This is the case, that can be solved analytically. Second, we plot the solution for the height of the bump equal to $\pi^2/2$. We see that there is a small change in the wave function. The energy is now higher (13.872 Ha). This is expected, since the particle is more confined.

(2) The way the wave function is plotted, the amplitude is in arbitrary units determined by the initial conditions (slope of the wave function at x=0). By normalizing the wave function as described in the text, we make sure that the probability of finding one electron in the double-well potential is exactly equal to one. The expectation value for the electron's coordinate is $<x>=0.5$. We could calculate this from the normalized wave function, but this can also be seen from symmetry reasons: The wave function needs to be symmetric with respect to x=0.5, since the potential has the same symmetry. We also see that the wave function is odd with respect to the symmetry axis (x=0.5). Wave functions for eigenstates with higher energies can be either odd or even, but the probability will always be even, since it is the absolute square of the wave function. We also see that the wave function is real, since there are no complex terms in the Schrödinger equation.

(3) For a height that is ten times higher ($5\pi^2$), the wave function is drastically different. The particle is now more likely confined in either of the two wells and less likely to be found where the bump is. However, there is still a large amount of leakage through the barrier, i.e., the particle can tunnel through the barrier (bump) between the two wells. The energy is now also much higher (45.76 Ha). If we increased the height of the bump even more, then the amplitude of the wave function would decrease where the barrier is and increase in the wells. The tunnelling rate between the two barriers would decrease.